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Structural dynamics and hole transfer in B-DNA: combining MD, RT-TDDFT and TB

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ABSTRACT

Hole transfer along DNA has implications in various fields, from nanotechnology to cell oxidative damage [1,2]. Computational approaches are particularly useful for this problem, to complement experimental data for interpretation of transfer mechanisms. To be predictive, computational results need to account for the inherent mobility of biological molecules during the time frame of experimental measurements. We address the structural variability of B-DNA and its effects on hole transfer in a combined molecular dynamics (MD), real-time time-dependent density functional theory (RT-TDDFT) and Tight-Binding (TB) study [3]. We show that the quantities which characterize charge transfer, i.e., the time-dependent dipole moment and hole population at different sites, are sensitive to structural changes that occur on the nanosecond time scale. We extend the range of physical properties for which such correlation has been observed, further establishing the fact that quantitative computational data on charge transfer properties should include statistical averages. We use the RT-TDDFT results to assess an efficient tight-binding method suitable for high-throughput predictions. We demonstrate that charge transfer, although affected by structural variability, on average, remains strong in AA and GG dimers.

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